bw | HPC – C5

Environment Module System

Introduction

- Module System: Hardly used on desktop systems
- Common on clusters

- Problem: multiple versions of the same software packages and libraries are installed on the cluster.

- Solution: module system

- Each software version is installed as separate module
- Load the version you want to use

Module Environment Overview

- Supplies software in several versions.

- Software can be used by loading modules.

`> module avail`	show all installed software packages
`> module avail compiler`	show all available compilers
`> module load <module>`	load a module in list
`> module unload <module>`	remove a module from list
`> module purge`	remove all modules
`> module list`	show all loaded modules
`> module show <module>`	show environment variables of module
`> module help <module>`	show usage information of module

module avail

```
$ module avail
chem/gaussview/5.0.9
. . .
compiler/intel/15.1
compiler/intel/16.0
compiler/intel/17.0
. . .
math/matlab/R2017b
. . .
```

- Software is organized in **categories:**
  - bio
  - cae
  - chem
  - compiler
  - devel
  - lib
  - math
  - mpi
  - numlib
  - phys
  - system

module load and list

```
$ icc –version
-bash: icc: command not found
$ module load compiler/intel
$ icc –version
icc (ICC) 14.0.4 20140805

$ module list
Currently Loaded Modulefiles:
  1) compiler/intel/14.0(default)



$ module load compiler/intel/13.1
ERROR:150: Module 'compiler/intel/13.1' conflicts with
the currently loaded module(s) 'compiler/intel/14.0'
```

module unload

```
$ module load compiler/intel/13.1
$ icc --version
icc (ICC) 13.1.3 20130607

$ module unload compiler/intel/13.1
$ module load compiler/intel/14.0

$ icc --version
icc (ICC) 14.0.4 20140805
```

module show

How does the module command work?

- load: changes some environment variables
- unload: removes these changes

```
$ module show compiler/intel/14.0
setenv        INTEL_VERSION 14.0.4
prepend-path PATH /opt/bwhpc/common/compiler/intel/compxe...
prepend-path LD_LIBRARY_PATH /opt/bwhpc/common/compiler/i...
.
.
.
```

module help

- Each module has a small help page
- Read it before you use the module the first time
- Contains cluster specific information
  Example: `$ module help compiler/intel/14.0`
  - Which MKL version should I use?
  - Which MPI version should I use?
  - What to do in case of problems?